



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:53 AM UTC

PDB ID : 1RT2 / pdb_00001rt2
Title : CRYSTAL STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE COM-
PLEXED WITH TNK-651
Authors : Ren, J.; Esnouf, R.; Hopkins, A.; Willcox, B.; Jones, Y.; Ross, C.; Stammers,
D.; Stuart, D.
Deposited on : 1996-03-16
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

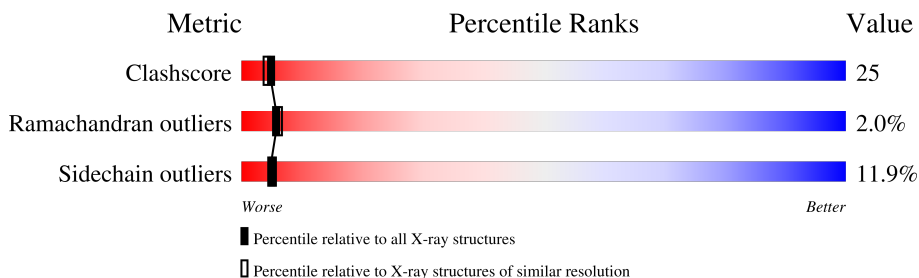
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	560	 43% 45% 7% . .
2	B	440	 40% 43% 8% 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7934 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	543	4435	2869	739	819	8	0	0	0

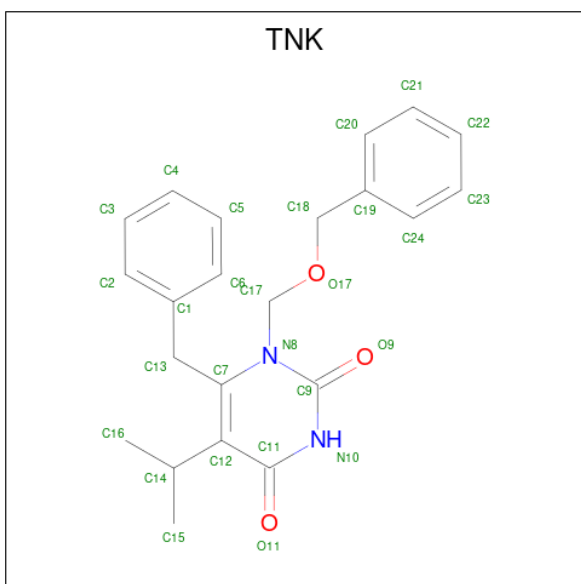
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	CSD	CYS	modified residue	UNP P04585

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	402	3334	2165	554	608	7	0	0	0

- Molecule 3 is 6-BENZYL-1-BENZYLOXYMETHYL-5-ISOPROPYL URACIL (CCD ID: TNK) (formula: C₂₂H₂₄N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	22	2	3	0	0

- Molecule 4 is water.

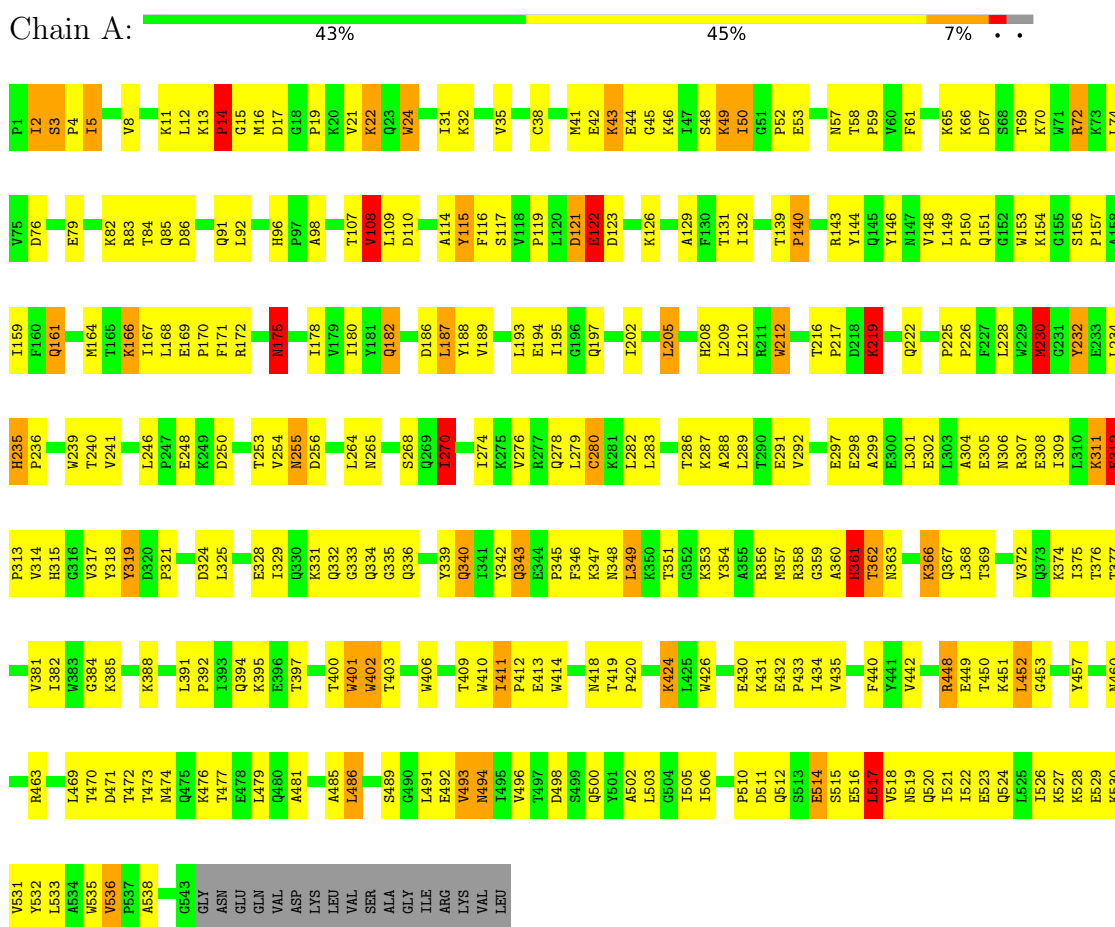
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	88	Total	O	0	0
			88	88		
4	B	50	Total	O	0	0
			50	50		

3 Residue-property plots

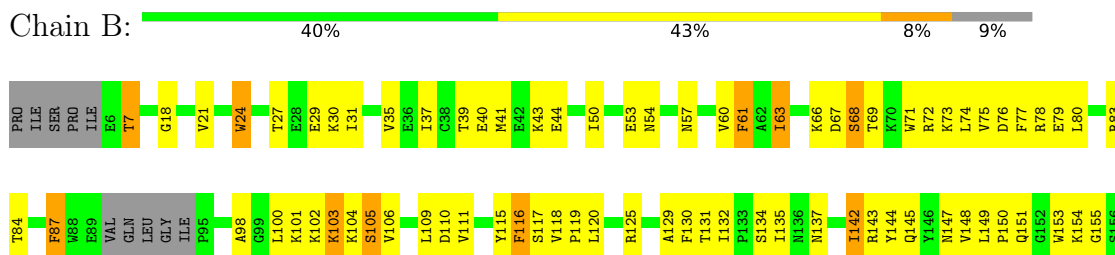
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

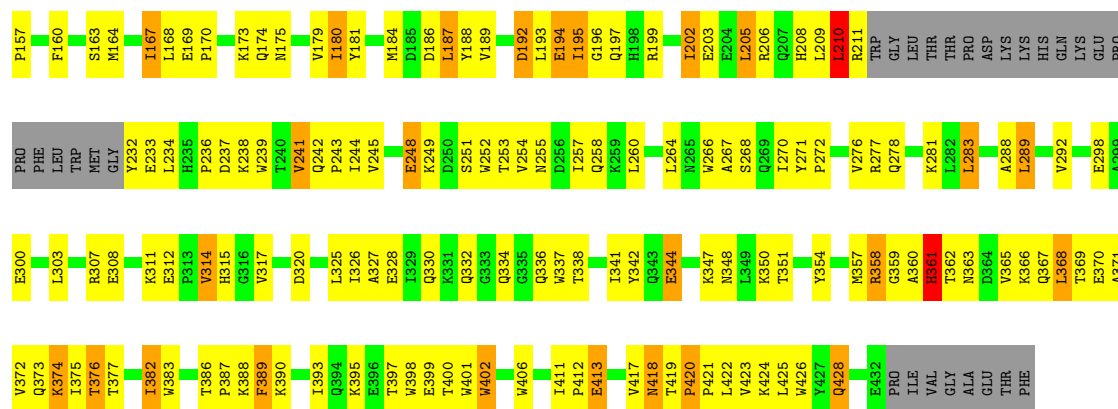
Note EDS was not executed.

- Molecule 1: HIV-1 REVERSE TRANSCRIPTASE



- Molecule 2: HIV-1 REVERSE TRANSCRIPTASE





4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	137.30Å 110.20Å 72.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.55	Depositor
% Data completeness (in resolution range)	85.3 (20.00-2.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.207 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7934	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, TNK

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.64	1/4544 (0.0%)	1.11	32/6175 (0.5%)
2	B	0.62	0/3426	1.08	24/4649 (0.5%)
All	All	0.64	1/7970 (0.0%)	1.09	56/10824 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	270	ILE	CA-CB	5.34	1.60	1.54

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	TYR	N-CA-C	8.23	122.04	108.96
1	A	349	LEU	N-CA-C	-8.08	101.54	111.40
1	A	494	ASN	N-CA-C	-8.05	95.79	109.24
1	A	388	LYS	N-CA-C	-8.03	96.97	109.25
1	A	312	GLU	CA-C-N	7.45	129.15	119.84
1	A	312	GLU	C-N-CA	7.45	129.15	119.84
1	A	50	ILE	N-CA-C	7.37	117.52	108.53
1	A	536	VAL	CA-C-N	7.26	127.02	119.76
1	A	536	VAL	C-N-CA	7.26	127.02	119.76
1	A	297	GLU	N-CA-C	-7.06	103.51	111.14
2	B	68	SER	N-CA-C	-6.67	96.17	107.99
2	B	87	PHE	N-CA-C	6.62	117.87	108.54
1	A	3	SER	N-CA-C	6.46	119.00	109.50
2	B	420	PRO	CA-C-N	6.43	127.88	119.84
2	B	420	PRO	C-N-CA	6.43	127.88	119.84
2	B	417	VAL	N-CA-C	6.40	116.34	108.53
1	A	382	ILE	N-CA-C	6.36	117.94	111.00
2	B	248	GLU	N-CA-C	-6.25	101.69	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	235	HIS	N-CA-C	-6.01	103.22	110.13
2	B	18	GLY	CA-C-N	5.88	126.07	119.90
2	B	18	GLY	C-N-CA	5.88	126.07	119.90
2	B	320	ASP	CA-C-N	5.86	126.27	119.47
2	B	320	ASP	C-N-CA	5.86	126.27	119.47
2	B	413	GLU	N-CA-C	-5.85	101.82	110.48
1	A	115	TYR	N-CA-C	-5.82	104.93	111.28
1	A	212	TRP	N-CA-C	5.80	120.05	113.15
2	B	205	LEU	N-CA-C	-5.78	104.61	111.03
1	A	187	LEU	N-CA-C	-5.78	97.74	108.02
1	A	517	LEU	N-CA-C	-5.78	104.89	111.07
1	A	411	ILE	N-CA-C	-5.70	100.83	107.61
2	B	210	LEU	N-CA-C	-5.59	98.90	110.80
1	A	216	THR	N-CA-C	5.56	116.66	109.65
2	B	344	GLU	N-CA-C	-5.54	101.59	109.62
2	B	382	ILE	N-CA-C	5.54	117.45	111.58
1	A	197	GLN	N-CA-C	-5.44	105.00	111.69
1	A	401	TRP	N-CA-C	5.41	117.03	111.03
1	A	411	ILE	CB-CA-C	-5.39	104.91	110.13
1	A	343	GLN	N-CA-C	-5.38	106.39	113.12
2	B	186	ASP	N-CA-C	5.35	118.00	110.14
1	A	175	ASN	CA-C-N	5.32	126.49	119.84
1	A	175	ASN	C-N-CA	5.32	126.49	119.84
1	A	44	GLU	N-CA-C	-5.29	106.52	112.87
2	B	389	PHE	N-CA-C	5.29	118.73	110.32
1	A	366	LYS	N-CA-C	-5.23	105.27	110.97
2	B	132	ILE	N-CA-C	-5.21	101.94	107.77
2	B	361	HIS	N-CA-C	5.18	121.84	110.80
2	B	175	ASN	CA-C-N	5.18	124.90	119.82
2	B	175	ASN	C-N-CA	5.18	124.90	119.82
1	A	531	VAL	CB-CA-C	-5.17	102.78	110.33
1	A	108	VAL	N-CA-C	5.17	115.02	107.37
2	B	402	TRP	N-CA-C	5.13	116.87	111.28
2	B	400	THR	N-CA-C	5.12	117.65	111.40
1	A	188	TYR	N-CA-C	-5.12	100.17	108.41
1	A	486	LEU	N-CA-C	5.08	116.90	111.36
1	A	361	HIS	N-CA-C	5.05	121.56	110.80
2	B	363	ASN	N-CA-C	5.01	117.11	107.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4435	0	4483	240	0
2	B	3334	0	3360	169	0
3	A	27	0	24	2	0
4	A	88	0	0	6	0
4	B	50	0	0	0	0
All	All	7934	0	7867	396	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 25.

All (396) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:GLU:HB3	2:B:390:LYS:HD3	1.48	0.94
1:A:241:VAL:HB	1:A:314:VAL:HG23	1.55	0.89
2:B:241:VAL:HG22	2:B:350:LYS:HG3	1.56	0.86
2:B:103:LYS:HE3	2:B:103:LYS:HA	1.58	0.85
1:A:491:LEU:HD12	1:A:529:GLU:HG3	1.60	0.83
1:A:270:ILE:HD11	1:A:314:VAL:HB	1.60	0.83
2:B:60:VAL:HG12	2:B:75:VAL:HG22	1.60	0.82
2:B:241:VAL:HG13	2:B:351:THR:H	1.42	0.82
1:A:115:TYR:HD2	1:A:156:SER:HB3	1.46	0.81
1:A:96:HIS:HD2	1:A:98:ALA:HB3	1.47	0.80
2:B:84:THR:HB	2:B:154:LYS:HE2	1.64	0.80
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.62	0.79
1:A:43:LYS:HE3	1:A:43:LYS:HA	1.65	0.78
2:B:115:TYR:HB3	2:B:149:LEU:HB2	1.65	0.77
2:B:164:MET:HE3	2:B:168:LEU:HD11	1.68	0.76
2:B:193:LEU:HB3	2:B:197:GLN:HB3	1.68	0.76
1:A:116:PHE:CE2	1:A:151:GLN:HG3	2.20	0.76
2:B:241:VAL:HG13	2:B:351:THR:N	2.02	0.75
1:A:57:ASN:HB2	1:A:143:ARG:HH22	1.52	0.74
1:A:49:LYS:HA	1:A:143:ARG:O	1.88	0.72
1:A:59:PRO:HG2	1:A:76:ASP:HB3	1.70	0.72
1:A:180:ILE:HG12	1:A:189:VAL:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:THR:HG22	1:A:315:HIS:HB3	1.72	0.70
1:A:402:TRP:CH2	2:B:362:THR:HA	2.26	0.70
1:A:19:PRO:HD3	1:A:83:ARG:HD2	1.74	0.70
1:A:8:VAL:O	1:A:121:ASP:HB2	1.91	0.69
2:B:24:TRP:NE1	2:B:61:PHE:HE2	1.90	0.69
2:B:120:LEU:HD23	2:B:125:ARG:HG2	1.76	0.68
1:A:96:HIS:CD2	1:A:98:ALA:HB3	2.28	0.68
1:A:278:GLN:O	1:A:282:LEU:HD13	1.94	0.68
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.27	0.68
2:B:7:THR:HG21	2:B:119:PRO:O	1.93	0.68
1:A:406:TRP:CH2	2:B:418:ASN:HA	2.29	0.68
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.75	0.67
2:B:244:ILE:HG13	2:B:426:TRP:CZ2	2.29	0.67
1:A:115:TYR:O	1:A:149:LEU:HB2	1.96	0.66
2:B:376:THR:HG23	2:B:387:PRO:HD2	1.77	0.66
1:A:442:VAL:HG11	1:A:485:ALA:HB2	1.78	0.66
1:A:450:THR:HB	1:A:452:LEU:HD23	1.76	0.66
2:B:368:LEU:O	2:B:372:VAL:HG23	1.96	0.66
1:A:426:TRP:HB3	1:A:526:ILE:HD13	1.78	0.65
2:B:332:GLN:HG3	2:B:338:THR:HG23	1.78	0.65
1:A:168:LEU:O	1:A:172:ARG:HG3	1.97	0.64
2:B:57:ASN:HD22	2:B:143:ARG:NH1	1.96	0.64
1:A:57:ASN:HA	1:A:129:ALA:O	1.98	0.64
2:B:105:SER:HA	2:B:234:LEU:O	1.96	0.64
1:A:149:LEU:HD21	1:A:159:ILE:HG21	1.79	0.64
1:A:246:LEU:HB2	1:A:307:ARG:NH1	2.13	0.63
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.81	0.63
2:B:398:TRP:O	2:B:402:TRP:HD1	1.81	0.63
1:A:24:TRP:CE3	1:A:61:PHE:HZ	2.16	0.63
1:A:232:TYR:HB3	1:A:240:THR:O	1.99	0.63
2:B:328:GLU:HB2	2:B:390:LYS:HB2	1.81	0.63
1:A:219:LYS:HD3	1:A:222:GLN:HG3	1.81	0.62
1:A:331:LYS:HE2	1:A:333:GLY:O	2.00	0.62
1:A:24:TRP:HE3	1:A:61:PHE:HZ	1.48	0.62
2:B:40:GLU:O	2:B:44:GLU:HG3	1.99	0.62
2:B:103:LYS:HE2	2:B:192:ASP:HB3	1.81	0.62
1:A:149:LEU:HD11	1:A:159:ILE:HG22	1.82	0.62
2:B:106:VAL:HA	2:B:189:VAL:O	2.00	0.62
2:B:360:ALA:HA	2:B:366:LYS:HD3	1.82	0.61
1:A:376:THR:HG21	2:B:401:TRP:HZ2	1.65	0.61
2:B:325:LEU:HD21	2:B:383:TRP:CE3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:433:PRO:HA	1:A:532:TYR:CD2	2.35	0.61
2:B:39:THR:O	2:B:43:LYS:HG2	1.99	0.61
2:B:358:ARG:H	2:B:358:ARG:HD3	1.66	0.61
2:B:116:PHE:HD1	2:B:117:SER:N	1.98	0.61
2:B:374:LYS:HB2	2:B:374:LYS:NZ	2.15	0.61
1:A:110:ASP:HB3	1:A:217:PRO:HB3	1.82	0.61
2:B:395:LYS:O	2:B:399:GLU:HG3	2.01	0.60
1:A:12:LEU:O	1:A:13:LYS:C	2.45	0.60
1:A:517:LEU:O	1:A:521:ILE:HG13	2.01	0.60
1:A:518:VAL:O	1:A:522:ILE:HG13	2.01	0.60
2:B:232:TYR:HD1	2:B:233:GLU:H	1.48	0.60
2:B:232:TYR:HD1	2:B:233:GLU:N	2.00	0.60
2:B:27:THR:HG22	2:B:29:GLU:HG2	1.83	0.59
2:B:328:GLU:CB	2:B:390:LYS:HB2	2.32	0.59
1:A:451:LYS:HB3	1:A:471:ASP:HA	1.84	0.59
2:B:337:TRP:HB2	2:B:354:TYR:HB3	1.83	0.59
2:B:101:LYS:HD2	2:B:382:ILE:HG23	1.84	0.59
2:B:30:LYS:NZ	2:B:71:TRP:HZ3	2.01	0.58
2:B:195:ILE:HG23	2:B:196:GLY:H	1.68	0.58
2:B:24:TRP:HE1	2:B:61:PHE:HE2	1.51	0.58
2:B:111:VAL:HG11	2:B:187:LEU:HD22	1.84	0.58
2:B:193:LEU:HB3	2:B:197:GLN:CB	2.33	0.58
1:A:182:GLN:HG2	1:A:187:LEU:HD23	1.85	0.57
1:A:246:LEU:HD23	1:A:307:ARG:HG2	1.86	0.57
1:A:426:TRP:HB3	1:A:526:ILE:CD1	2.34	0.57
1:A:157:PRO:O	1:A:161:GLN:HB2	2.05	0.57
1:A:5:ILE:HD13	1:A:167:ILE:HD11	1.87	0.57
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.86	0.57
2:B:169:GLU:O	2:B:173:LYS:HD3	2.05	0.57
1:A:453:GLY:HA3	1:A:472:THR:CG2	2.35	0.57
1:A:115:TYR:CD2	1:A:156:SER:HB3	2.35	0.56
2:B:160:PHE:O	2:B:164:MET:HB2	2.05	0.56
1:A:264:LEU:HD12	1:A:274:ILE:HG23	1.87	0.56
1:A:517:LEU:HA	1:A:520:GLN:OE1	2.05	0.56
2:B:142:ILE:HG22	2:B:144:TYR:CE2	2.39	0.56
2:B:308:GLU:O	2:B:311:LYS:HB2	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
2:B:270:ILE:O	2:B:272:PRO:HD3	2.05	0.56
1:A:419:THR:HG21	4:A:1062:HOH:O	2.05	0.56
2:B:360:ALA:HB1	2:B:367:GLN:HG3	1.88	0.56
1:A:167:ILE:HG23	1:A:212:TRP:CD1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:TRP:CH2	2:B:362:THR:HG23	2.41	0.56
2:B:167:ILE:O	2:B:208:HIS:HE1	1.89	0.56
1:A:239:TRP:O	1:A:315:HIS:HB2	2.06	0.55
1:A:306:ASN:HA	1:A:309:ILE:HG22	1.89	0.55
2:B:27:THR:CG2	2:B:29:GLU:HG2	2.36	0.55
2:B:79:GLU:O	2:B:83:ARG:HG3	2.05	0.55
1:A:248:GLU:HB2	4:A:1046:HOH:O	2.06	0.55
1:A:520:GLN:O	1:A:523:GLU:HB2	2.06	0.55
1:A:69:THR:O	1:A:69:THR:HG22	2.06	0.54
2:B:253:THR:O	2:B:257:ILE:HG12	2.07	0.54
2:B:373:GLN:O	2:B:377:THR:HG23	2.06	0.54
1:A:253:THR:HG22	1:A:292:VAL:HG22	1.88	0.54
1:A:402:TRP:HH2	2:B:362:THR:HA	1.73	0.54
1:A:424:LYS:NZ	1:A:424:LYS:HB3	2.22	0.54
1:A:486:LEU:HB3	1:A:524:GLN:HB3	1.88	0.54
2:B:7:THR:HG23	2:B:119:PRO:HG2	1.90	0.54
1:A:331:LYS:CE	1:A:334:GLN:HA	2.38	0.54
2:B:374:LYS:HB2	2:B:374:LYS:HZ2	1.72	0.53
2:B:317:VAL:HG22	2:B:347:LYS:HD2	1.91	0.53
1:A:442:VAL:CG1	1:A:485:ALA:HB2	2.38	0.53
2:B:154:LYS:O	2:B:157:PRO:HD2	2.08	0.53
1:A:287:LYS:HG2	1:A:291:GLU:CD	2.33	0.53
1:A:340:GLN:HB2	1:A:351:THR:HG22	1.89	0.53
2:B:357:MET:O	2:B:359:GLY:N	2.42	0.53
1:A:46:LYS:HD2	1:A:116:PHE:HB3	1.90	0.53
1:A:514:GLU:HG3	1:A:515:SER:H	1.74	0.53
1:A:516:GLU:HA	1:A:519:ASN:HD22	1.72	0.53
2:B:120:LEU:HB2	2:B:148:VAL:O	2.09	0.52
2:B:248:GLU:HG2	2:B:307:ARG:HH12	1.74	0.52
1:A:58:THR:HG23	1:A:59:PRO:HD2	1.90	0.52
1:A:376:THR:HG21	2:B:401:TRP:CZ2	2.44	0.52
1:A:167:ILE:O	1:A:170:PRO:HD2	2.08	0.52
2:B:54:ASN:HD21	2:B:129:ALA:HB2	1.74	0.52
2:B:73:LYS:NZ	2:B:130:PHE:CZ	2.76	0.52
2:B:173:LYS:HD2	2:B:173:LYS:N	2.24	0.52
2:B:398:TRP:O	2:B:402:TRP:CD1	2.62	0.52
2:B:30:LYS:NZ	2:B:71:TRP:CZ3	2.77	0.52
2:B:87:PHE:CE2	2:B:155:GLY:HA2	2.45	0.52
2:B:277:ARG:HG3	2:B:278:GLN:H	1.73	0.52
1:A:70:LYS:HE3	1:A:72:ARG:NH1	2.24	0.52
2:B:366:LYS:HE2	2:B:370:GLU:OE2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:HD12	1:A:148:VAL:CG1	2.40	0.52
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.91	0.52
1:A:523:GLU:O	1:A:527:LYS:HG2	2.10	0.51
2:B:249:LYS:HB3	2:B:252:TRP:CE2	2.46	0.51
2:B:388:LYS:HG2	2:B:413:GLU:HB3	1.91	0.51
1:A:331:LYS:HE2	1:A:334:GLN:HA	1.93	0.51
1:A:329:ILE:HD11	1:A:375:ILE:HD12	1.92	0.51
1:A:498:ASP:HA	1:A:536:VAL:O	2.10	0.51
2:B:267:ALA:HB2	2:B:426:TRP:CZ3	2.46	0.51
2:B:142:ILE:N	2:B:142:ILE:HD12	2.26	0.51
1:A:479:LEU:HB3	1:A:521:ILE:HD11	1.93	0.51
1:A:8:VAL:HG13	2:B:53:GLU:OE1	2.11	0.51
2:B:266:TRP:CZ2	2:B:423:VAL:HG22	2.46	0.51
1:A:86:ASP:HA	1:A:154:LYS:HZ1	1.76	0.50
1:A:360:ALA:HA	1:A:514:GLU:HB3	1.92	0.50
1:A:278:GLN:HB3	1:A:299:ALA:HA	1.93	0.50
1:A:278:GLN:HG2	1:A:298:GLU:C	2.36	0.50
2:B:77:PHE:CD1	2:B:80:LEU:HD23	2.47	0.50
2:B:142:ILE:HD12	2:B:142:ILE:H	1.75	0.50
1:A:57:ASN:HB2	1:A:143:ARG:NH2	2.22	0.50
1:A:178:ILE:HD11	1:A:193:LEU:HD11	1.93	0.50
1:A:301:LEU:O	1:A:304:ALA:HB3	2.12	0.50
1:A:194:GLU:CD	1:A:194:GLU:H	2.20	0.50
1:A:361:HIS:HB2	1:A:510:PRO:HB3	1.93	0.50
2:B:342:TYR:HB3	2:B:348:ASN:HA	1.94	0.50
1:A:331:LYS:HE2	1:A:333:GLY:C	2.37	0.49
1:A:276:VAL:O	1:A:280:CSD:HB3	2.12	0.49
1:A:519:ASN:O	1:A:523:GLU:HG2	2.12	0.49
2:B:314:VAL:HG22	2:B:315:HIS:O	2.12	0.49
2:B:317:VAL:HG13	2:B:347:LYS:HB3	1.94	0.49
1:A:182:GLN:HG2	1:A:187:LEU:CD2	2.42	0.49
1:A:254:VAL:HB	1:A:289:LEU:HA	1.94	0.49
1:A:21:VAL:HG11	1:A:59:PRO:HD3	1.94	0.49
1:A:311:LYS:HE3	1:A:311:LYS:O	2.12	0.49
1:A:418:ASN:O	1:A:420:PRO:HD3	2.12	0.49
2:B:372:VAL:O	2:B:376:THR:OG1	2.28	0.49
2:B:252:TRP:CZ3	2:B:260:LEU:HD22	2.48	0.49
1:A:228:LEU:HD12	1:A:228:LEU:N	2.28	0.49
1:A:360:ALA:HA	1:A:514:GLU:HG2	1.94	0.49
1:A:361:HIS:HA	1:A:512:GLN:O	2.13	0.49
1:A:369:THR:HG21	1:A:409:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLU:HG3	1:A:515:SER:N	2.28	0.49
2:B:103:LYS:O	2:B:236:PRO:HD2	2.12	0.49
1:A:448:ARG:HE	1:A:474:ASN:HB2	1.78	0.48
2:B:76:ASP:HA	2:B:411:ILE:HD12	1.95	0.48
1:A:79:GLU:OE2	1:A:82:LYS:HD3	2.13	0.48
1:A:253:THR:O	1:A:256:ASP:HB2	2.13	0.48
1:A:450:THR:HB	1:A:452:LEU:CD2	2.43	0.48
2:B:327:ALA:O	2:B:389:PHE:HA	2.13	0.48
1:A:372:VAL:HG11	1:A:411:ILE:HG23	1.96	0.48
1:A:430:GLU:HG2	4:A:1068:HOH:O	2.14	0.48
1:A:457:TYR:HE1	1:A:463:ARG:HG2	1.78	0.48
1:A:178:ILE:HD11	1:A:193:LEU:CD1	2.44	0.48
2:B:150:PRO:HD2	2:B:153:TRP:CE3	2.49	0.48
2:B:205:LEU:O	2:B:208:HIS:HB3	2.14	0.48
1:A:79:GLU:HA	1:A:82:LYS:HG2	1.96	0.48
1:A:384:GLY:CA	2:B:135:ILE:HD12	2.44	0.48
1:A:498:ASP:HB2	1:A:538:ALA:HB2	1.95	0.48
1:A:279:LEU:HD23	1:A:302:GLU:OE2	2.13	0.48
2:B:248:GLU:HA	2:B:307:ARG:HH22	1.79	0.48
1:A:278:GLN:HG2	1:A:299:ALA:N	2.28	0.48
1:A:502:ALA:HA	1:A:505:ILE:HD12	1.94	0.48
2:B:237:ASP:C	2:B:239:TRP:H	2.21	0.48
1:A:402:TRP:CZ2	2:B:362:THR:HA	2.49	0.47
1:A:535:TRP:CZ3	2:B:422:LEU:HD21	2.49	0.47
1:A:150:PRO:HG2	1:A:153:TRP:CB	2.44	0.47
1:A:516:GLU:O	1:A:520:GLN:HG3	2.15	0.47
2:B:103:LYS:C	2:B:105:SER:H	2.23	0.47
1:A:298:GLU:H	1:A:298:GLU:CD	2.22	0.47
1:A:406:TRP:CE3	2:B:419:THR:HB	2.49	0.47
1:A:359:GLY:C	1:A:361:HIS:N	2.72	0.47
1:A:448:ARG:HH21	1:A:474:ASN:HB3	1.80	0.47
1:A:270:ILE:HG13	1:A:270:ILE:O	2.13	0.47
1:A:413:GLU:HG2	4:A:1065:HOH:O	2.14	0.47
2:B:371:ALA:O	2:B:375:ILE:HG13	2.15	0.47
1:A:448:ARG:NH1	1:A:473:THR:HB	2.29	0.46
2:B:125:ARG:HD3	2:B:147:ASN:HA	1.95	0.46
1:A:334:GLN:HG2	1:A:356:ARG:NH2	2.31	0.46
1:A:11:LYS:O	1:A:85:GLN:HB3	2.15	0.46
2:B:421:PRO:O	2:B:425:LEU:HG	2.15	0.46
2:B:103:LYS:HA	2:B:103:LYS:CE	2.40	0.46
2:B:163:SER:O	2:B:167:ILE:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:TYR:CD1	2:B:233:GLU:N	2.83	0.46
2:B:278:GLN:HE21	2:B:298:GLU:HB3	1.80	0.46
1:A:96:HIS:CD2	1:A:98:ALA:CB	2.97	0.46
1:A:334:GLN:HG2	1:A:356:ARG:HH21	1.80	0.46
2:B:61:PHE:CD1	2:B:74:LEU:HD23	2.51	0.46
1:A:345:PRO:O	1:A:346:PHE:HB2	2.14	0.46
2:B:100:LEU:HD22	2:B:181:TYR:HB2	1.98	0.46
2:B:376:THR:HG22	2:B:386:THR:HG22	1.97	0.46
1:A:306:ASN:HA	1:A:309:ILE:CG2	2.45	0.46
1:A:340:GLN:CB	1:A:351:THR:HG22	2.46	0.46
1:A:363:ASN:HD21	1:A:401:TRP:HZ2	1.64	0.46
2:B:249:LYS:HG2	2:B:251:SER:O	2.15	0.46
1:A:225:PRO:HA	1:A:226:PRO:C	2.41	0.46
1:A:274:ILE:HD13	1:A:309:ILE:HD13	1.97	0.46
1:A:354:TYR:HE2	1:A:375:ILE:HG13	1.81	0.45
1:A:108:VAL:HG23	1:A:186:ASP:HB3	1.97	0.45
1:A:255:ASN:HD22	1:A:255:ASN:HA	1.56	0.45
1:A:394:GLN:HB2	1:A:397:THR:OG1	2.15	0.45
2:B:254:VAL:O	2:B:258:GLN:HG3	2.17	0.45
1:A:13:LYS:HA	1:A:85:GLN:HA	1.98	0.45
1:A:41:MET:CE	1:A:46:LYS:HE3	2.46	0.45
2:B:37:ILE:O	2:B:41:MET:HG3	2.16	0.45
1:A:12:LEU:O	1:A:14:PRO:N	2.49	0.45
1:A:48:SER:O	1:A:144:TYR:HA	2.16	0.45
1:A:328:GLU:HB3	1:A:340:GLN:OE1	2.16	0.45
1:A:301:LEU:O	1:A:305:GLU:HG3	2.16	0.45
2:B:268:SER:HA	2:B:271:TYR:O	2.16	0.45
1:A:122:GLU:H	1:A:122:GLU:CD	2.25	0.45
2:B:118:VAL:HA	2:B:119:PRO:HD2	1.86	0.45
1:A:328:GLU:O	1:A:339:TYR:HA	2.17	0.45
1:A:516:GLU:HA	1:A:519:ASN:ND2	2.32	0.45
2:B:57:ASN:ND2	2:B:131:THR:OG1	2.50	0.45
2:B:106:VAL:CG1	2:B:188:TYR:HB3	2.47	0.45
2:B:199:ARG:O	2:B:202:ILE:HG22	2.17	0.45
1:A:360:ALA:O	1:A:361:HIS:HB3	2.17	0.45
1:A:505:ILE:HG23	1:A:510:PRO:HD2	1.98	0.45
1:A:362:THR:HG22	1:A:366:LYS:HG2	1.98	0.45
1:A:524:GLN:O	1:A:528:LYS:HG2	2.17	0.44
1:A:53:GLU:O	1:A:53:GLU:HG2	2.18	0.44
1:A:123:ASP:O	1:A:126:LYS:HE3	2.16	0.44
3:A:999:TNK:H172	3:A:999:TNK:H131	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:TYR:HB2	1:A:151:GLN:NE2	2.32	0.44
1:A:166:LYS:O	1:A:169:GLU:HB3	2.16	0.44
2:B:311:LYS:O	2:B:312:GLU:HG3	2.18	0.44
1:A:43:LYS:C	1:A:45:GLY:N	2.75	0.44
1:A:114:ALA:HA	1:A:117:SER:HB2	1.99	0.44
1:A:319:TYR:CE1	1:A:343:GLN:NE2	2.85	0.44
1:A:460:ASN:ND2	2:B:288:ALA:HB2	2.32	0.44
2:B:365:VAL:O	2:B:369:THR:HG23	2.18	0.44
1:A:377:THR:O	1:A:381:VAL:HG23	2.17	0.44
1:A:384:GLY:HA3	2:B:135:ILE:HD12	1.99	0.44
2:B:424:LYS:NZ	2:B:428:GLN:HG3	2.32	0.44
1:A:114:ALA:HA	1:A:117:SER:OG	2.18	0.44
1:A:114:ALA:HA	1:A:117:SER:CB	2.48	0.44
1:A:342:TYR:HA	1:A:349:LEU:HG	1.98	0.44
1:A:472:THR:OG1	1:A:476:LYS:HB2	2.18	0.44
1:A:511:ASP:HA	1:A:522:ILE:HD13	2.00	0.44
1:A:17:ASP:O	1:A:83:ARG:HD3	2.18	0.44
1:A:248:GLU:HB3	1:A:307:ARG:NH2	2.33	0.44
1:A:522:ILE:O	1:A:526:ILE:HG13	2.18	0.44
1:A:460:ASN:HD22	2:B:288:ALA:HB2	1.83	0.43
1:A:58:THR:CG2	1:A:59:PRO:HD2	2.48	0.43
2:B:72:ARG:HH22	2:B:110:ASP:CG	2.26	0.43
1:A:65:LYS:C	1:A:67:ASP:H	2.26	0.43
1:A:270:ILE:HG12	1:A:314:VAL:HG21	2.00	0.43
1:A:317:VAL:HG22	1:A:318:TYR:H	1.82	0.43
2:B:180:ILE:HA	2:B:188:TYR:O	2.18	0.43
2:B:248:GLU:HG2	2:B:307:ARG:NH1	2.34	0.43
2:B:72:ARG:NH2	2:B:151:GLN:OE1	2.52	0.43
2:B:194:GLU:O	2:B:197:GLN:HB2	2.18	0.43
1:A:16:MET:HB3	1:A:17:ASP:H	1.69	0.43
2:B:277:ARG:HG3	2:B:278:GLN:N	2.32	0.43
2:B:420:PRO:HA	2:B:421:PRO:HD3	1.78	0.43
1:A:22:LYS:HG2	4:A:1002:HOH:O	2.18	0.43
1:A:329:ILE:O	1:A:392:PRO:HD3	2.19	0.43
2:B:210:LEU:O	2:B:211:ARG:CB	2.66	0.43
1:A:3:SER:HB3	1:A:5:ILE:HG13	1.99	0.43
1:A:503:LEU:HA	1:A:506:ILE:HD12	2.00	0.43
2:B:180:ILE:HG22	2:B:187:LEU:HG	2.01	0.43
2:B:195:ILE:HG23	2:B:196:GLY:N	2.32	0.43
1:A:119:PRO:HA	1:A:148:VAL:HA	2.01	0.42
1:A:527:LYS:HE2	1:A:527:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ILE:O	2:B:35:VAL:HG23	2.19	0.42
1:A:332:GLN:HE22	1:A:353:LYS:NZ	2.17	0.42
2:B:205:LEU:O	2:B:209:LEU:HG	2.20	0.42
2:B:388:LYS:HG2	2:B:413:GLU:CB	2.48	0.42
1:A:319:TYR:OH	1:A:385:LYS:NZ	2.49	0.42
1:A:520:GLN:HA	1:A:523:GLU:HG2	2.00	0.42
2:B:358:ARG:O	2:B:358:ARG:HG2	2.20	0.42
1:A:107:THR:N	1:A:189:VAL:O	2.49	0.42
1:A:205:LEU:O	1:A:209:LEU:HG	2.20	0.42
1:A:426:TRP:O	1:A:526:ILE:HG23	2.20	0.42
2:B:197:GLN:NE2	2:B:197:GLN:HA	2.34	0.42
2:B:393:ILE:HD13	2:B:398:TRP:HE3	1.84	0.42
1:A:307:ARG:HD2	4:A:1048:HOH:O	2.20	0.42
2:B:195:ILE:HD11	2:B:199:ARG:NH2	2.34	0.42
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.67	0.42
1:A:432:GLU:OE1	1:A:433:PRO:HD2	2.19	0.42
2:B:111:VAL:CG1	2:B:187:LEU:HD22	2.49	0.42
1:A:335:GLY:HA2	1:A:367:GLN:OE1	2.20	0.42
1:A:361:HIS:HB2	1:A:510:PRO:CB	2.50	0.42
1:A:434:ILE:HD12	1:A:493:VAL:O	2.19	0.42
2:B:120:LEU:HB2	2:B:148:VAL:C	2.44	0.42
2:B:326:ILE:O	2:B:341:ILE:HA	2.19	0.42
1:A:21:VAL:CG1	1:A:59:PRO:HD3	2.50	0.41
1:A:434:ILE:HD13	1:A:530:LYS:HB3	2.02	0.41
1:A:440:PHE:CE1	1:A:489:SER:HB3	2.55	0.41
3:A:999:TNK:H163	3:A:999:TNK:O11	2.19	0.41
2:B:249:LYS:HE2	2:B:249:LYS:HB2	1.88	0.41
1:A:38:CYS:SG	1:A:132:ILE:HD11	2.60	0.41
1:A:79:GLU:O	1:A:83:ARG:NH1	2.53	0.41
1:A:205:LEU:O	1:A:208:HIS:HB3	2.21	0.41
1:A:442:VAL:HB	1:A:481:ALA:HB1	2.01	0.41
2:B:50:ILE:HG21	2:B:145:GLN:CB	2.49	0.41
1:A:57:ASN:HD22	1:A:143:ARG:CZ	2.33	0.41
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.03	0.41
2:B:35:VAL:O	2:B:39:THR:HG23	2.21	0.41
2:B:63:ILE:CD1	2:B:74:LEU:HB2	2.50	0.41
2:B:77:PHE:O	2:B:78:ARG:C	2.63	0.41
2:B:289:LEU:HA	2:B:289:LEU:HD12	1.76	0.41
1:A:150:PRO:HG2	1:A:153:TRP:HB2	2.03	0.41
2:B:163:SER:O	2:B:167:ILE:HG23	2.20	0.41
2:B:242:GLN:NE2	2:B:243:PRO:HD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:O	1:A:83:ARG:HG2	2.20	0.41
1:A:340:GLN:HA	1:A:351:THR:HA	2.02	0.41
2:B:134:SER:OG	2:B:137:ASN:HA	2.20	0.41
2:B:255:ASN:O	2:B:258:GLN:HB2	2.21	0.41
2:B:359:GLY:O	2:B:361:HIS:CD2	2.74	0.41
1:A:86:ASP:HA	1:A:154:LYS:NZ	2.35	0.41
1:A:96:HIS:CD2	1:A:98:ALA:H	2.38	0.41
1:A:278:GLN:HG2	1:A:298:GLU:HB2	2.02	0.41
1:A:312:GLU:HA	1:A:313:PRO:HD3	1.65	0.41
1:A:489:SER:HB2	1:A:493:VAL:HG13	2.02	0.41
2:B:344:GLU:HB3	2:B:347:LYS:HB2	2.03	0.41
1:A:84:THR:HB	1:A:154:LYS:HD3	2.03	0.41
1:A:319:TYR:HE1	1:A:343:GLN:NE2	2.18	0.41
2:B:142:ILE:CG2	2:B:144:TYR:CE2	3.02	0.41
1:A:164:MET:O	1:A:168:LEU:HG	2.20	0.41
2:B:125:ARG:O	2:B:145:GLN:HG3	2.19	0.41
2:B:181:TYR:O	2:B:187:LEU:HA	2.21	0.41
2:B:420:PRO:HB2	2:B:423:VAL:HG23	2.02	0.41
1:A:372:VAL:O	1:A:375:ILE:HB	2.21	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.41
2:B:406:TRP:CH2	2:B:412:PRO:HD3	2.56	0.41
1:A:92:LEU:HD13	1:A:92:LEU:HA	1.87	0.41
1:A:412:PRO:O	1:A:414:TRP:HD1	2.03	0.41
1:A:413:GLU:O	1:A:413:GLU:HG3	2.21	0.41
2:B:266:TRP:CH2	2:B:423:VAL:HG13	2.55	0.41
2:B:281:LYS:C	2:B:283:LEU:H	2.29	0.41
1:A:15:GLY:O	1:A:16:MET:HG3	2.22	0.40
2:B:157:PRO:HB3	2:B:184:MET:O	2.21	0.40
2:B:206:ARG:O	2:B:209:LEU:HB2	2.21	0.40
2:B:330:GLN:HB2	2:B:338:THR:OG1	2.21	0.40
1:A:139:THR:HA	1:A:140:PRO:HD2	1.90	0.40
1:A:156:SER:HB2	1:A:157:PRO:HD3	2.03	0.40
1:A:230:MET:SD	1:A:230:MET:N	2.94	0.40
1:A:265:ASN:O	1:A:268:SER:HB2	2.21	0.40
1:A:319:TYR:O	1:A:321:PRO:HD3	2.20	0.40
1:A:360:ALA:HA	1:A:514:GLU:CB	2.51	0.40
1:A:171:PHE:O	1:A:175:ASN:ND2	2.55	0.40
1:A:235:HIS:HB3	1:A:236:PRO:HD2	2.03	0.40
1:A:264:LEU:HD12	1:A:274:ILE:CG2	2.50	0.40
1:A:329:ILE:HD12	1:A:391:LEU:CD2	2.51	0.40
1:A:50:ILE:HG13	1:A:143:ARG:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:170:PRO:CD	2.44	0.40
1:A:342:TYR:HB2	1:A:347:LYS:O	2.22	0.40
2:B:66:LYS:C	2:B:68:SER:H	2.29	0.40
1:A:31:ILE:O	1:A:35:VAL:HG23	2.21	0.40
1:A:57:ASN:ND2	1:A:131:THR:OG1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	540/560 (96%)	464 (86%)	64 (12%)	12 (2%)	5	5
2	B	396/440 (90%)	343 (87%)	46 (12%)	7 (2%)	6	7
All	All	936/1000 (94%)	807 (86%)	110 (12%)	19 (2%)	6	6

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	PRO
1	A	122	GLU
1	A	230	MET
2	B	361	HIS
2	B	358	ARG
1	A	91	GLN
1	A	121	ASP
1	A	219	LYS
2	B	67	ASP
2	B	210	LEU
1	A	140	PRO
1	A	361	HIS
1	A	448	ARG

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Mol	Chain	Res	Type
2	B	98	ALA
2	B	195	ILE
1	A	288	ALA
1	A	52	PRO
2	B	241	VAL
1	A	195	ILE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	485/499 (97%)	425 (88%)	60 (12%)	4	4
2	B	367/400 (92%)	326 (89%)	41 (11%)	6	6
All	All	852/899 (95%)	751 (88%)	101 (12%)	5	5

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	4	PRO
1	A	5	ILE
1	A	14	PRO
1	A	22	LYS
1	A	24	TRP
1	A	32	LYS
1	A	42	GLU
1	A	43	LYS
1	A	49	LYS
1	A	66	LYS
1	A	72	ARG
1	A	74	LEU
1	A	108	VAL
1	A	109	LEU
1	A	122	GLU
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	166	LYS
1	A	175	ASN
1	A	182	GLN
1	A	202	ILE
1	A	205	LEU
1	A	210	LEU
1	A	219	LYS
1	A	230	MET
1	A	232	TYR
1	A	234	LEU
1	A	250	ASP
1	A	255	ASN
1	A	270	ILE
1	A	283	LEU
1	A	286	THR
1	A	308	GLU
1	A	311	LYS
1	A	312	GLU
1	A	324	ASP
1	A	325	LEU
1	A	336	GLN
1	A	340	GLN
1	A	357	MET
1	A	358	ARG
1	A	362	THR
1	A	368	LEU
1	A	374	LYS
1	A	400	THR
1	A	402	TRP
1	A	403	THR
1	A	410	TRP
1	A	424	LYS
1	A	431	LYS
1	A	435	VAL
1	A	449	GLU
1	A	452	LEU
1	A	470	THR
1	A	493	VAL
1	A	496	VAL
1	A	500	GLN
1	A	514	GLU
1	A	517	LEU

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Mol	Chain	Res	Type
1	A	533	LEU
2	B	7	THR
2	B	21	VAL
2	B	24	TRP
2	B	61	PHE
2	B	63	ILE
2	B	69	THR
2	B	102	LYS
2	B	103	LYS
2	B	104	LYS
2	B	105	SER
2	B	109	LEU
2	B	116	PHE
2	B	142	ILE
2	B	167	ILE
2	B	174	GLN
2	B	179	VAL
2	B	180	ILE
2	B	187	LEU
2	B	192	ASP
2	B	194	GLU
2	B	202	ILE
2	B	203	GLU
2	B	238	LYS
2	B	245	VAL
2	B	264	LEU
2	B	276	VAL
2	B	283	LEU
2	B	289	LEU
2	B	292	VAL
2	B	300	GLU
2	B	303	LEU
2	B	314	VAL
2	B	334	GLN
2	B	336	GLN
2	B	361	HIS
2	B	368	LEU
2	B	374	LYS
2	B	376	THR
2	B	397	THR
2	B	418	ASN
2	B	428	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	96	HIS
1	A	174	GLN
1	A	175	ASN
1	A	222	GLN
1	A	242	GLN
1	A	255	ASN
1	A	258	GLN
1	A	332	GLN
1	A	500	GLN
2	B	57	ASN
2	B	161	GLN
2	B	182	GLN
2	B	197	GLN
2	B	207	GLN
2	B	208	HIS
2	B	242	GLN
2	B	255	ASN
2	B	278	GLN
2	B	334	GLN
2	B	336	GLN
2	B	361	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	CSD	A	280	1	4,7,8	0.81	0	1,8,10	5.15	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSD	A	280	1	-	2/2/6/8	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	CSD	OD1-SG-CB	5.15	115.08	105.60

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	280	CSD	N-CA-CB-SG
1	A	280	CSD	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	280	CSD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	TNK	A	999	-	29,29,29	0.84	1 (3%)	32,39,39	0.75	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TNK	A	999	-	-	4/14/14/14	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	TNK	C11-C12	2.14	1.48	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	TNK	O17-C17-N8-C7
3	A	999	TNK	O17-C17-N8-C9
3	A	999	TNK	N8-C17-O17-C18
3	A	999	TNK	C19-C18-O17-C17

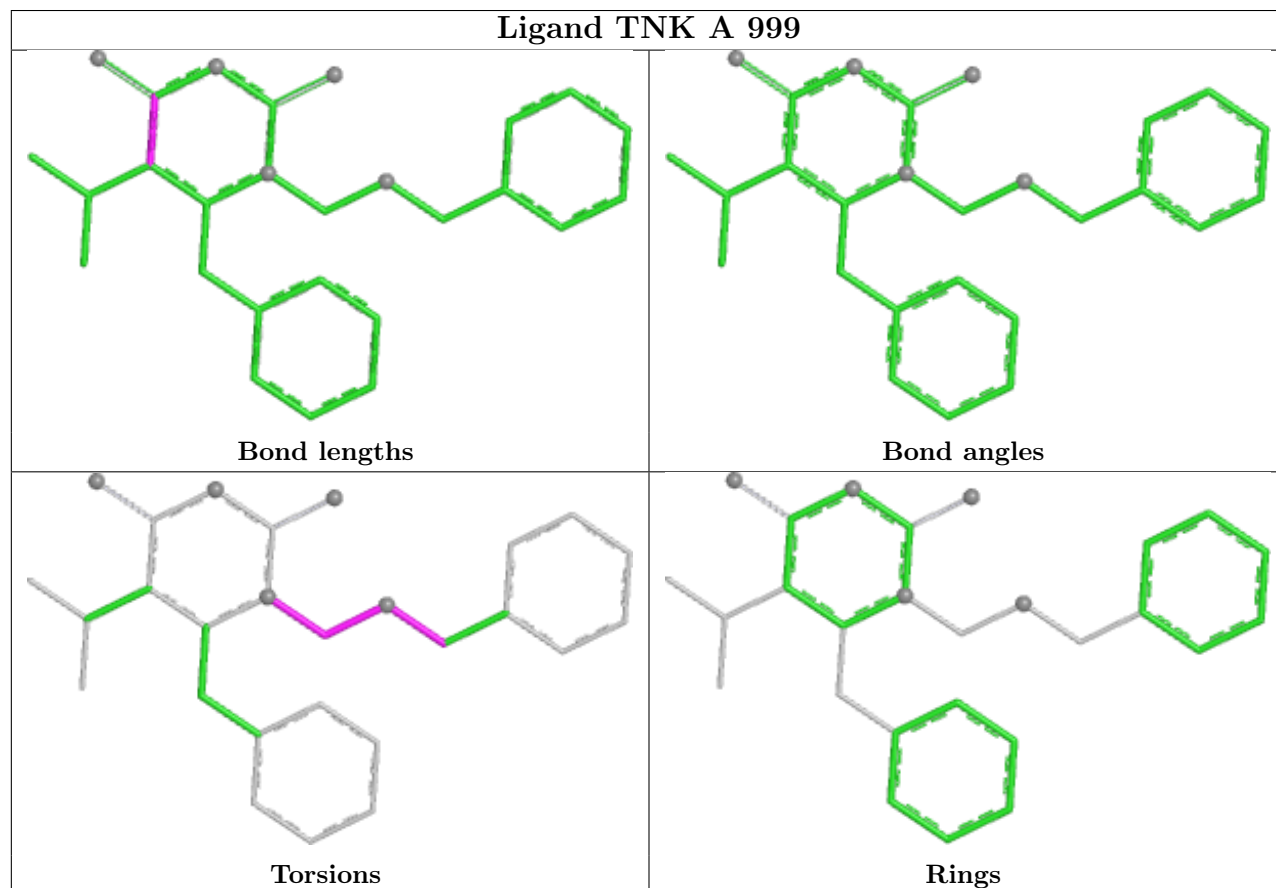
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	TNK	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.